Local Structure Study of V_2O_3

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Introduction: Vanadium sesquioxide undergoes a phase transition at 155K~165K from an antiferromagnetic insulator to paramagnetic metal with the crystal structure changing from monoclinic (I2/a) to trigonal (R3C)) with a 1.4% decrease in volume at elevated temperature. The metal-insulator transition in V_2O_3 is generally believed to be driven by the Mott-Hubbard (MH) mechanism, and indeed V_2O_3 is nowadays used as the best-studied example of a Mott Hubbard system with a metal-insulator transition. In this model, changes in V-V distances regulate the balance between the positive intra-atomic Coulomb repulsion energy of the electrons and their bare band energy width W by changing the overlap between 3d V-V orbital, thus determining the energy bandgap. According to diffraction measurement of the average structure, the monoclinic to trigonal phase transformation results in the decrease of V-V distances by about 0.11 A. However, recent experiments show there is still controversy with the metal-insulator transition model. M.L. denBoer *et al*. used x-ray absorption and photoemission spectroscopy to study the electronic structure of pure V_2O_3 above and below the metal-insulator transition temperature. [1] The result shows that although they are structurally different, the electronic structure of the trigonal V_2O_3 and monoclinic insulating V_2O_3 is essentially the same and they conclude there is no obvious symmetry breaking in the MIT. It should be emphasized that since the MH mechanism depends on the distance between the first few neighboring atoms and the corresponding overlap of their wave functions, the measurements of the local structure may help to determine whether this or some other mechanism holds. In A.I. Frenkel's paper, [2] the polarized XAFS measurements of the local structure of the single crystal V_2O_3 show the decrease in the volume but no change in local symmetry in the transition. The result indicated that the phase transition contained a significant order – disorder component, which is contrary to the purely displace model based on diffraction results. In this experiment, Rietveld refinement is performed to get the average structure and pair-distribution function (PDF) to get the local structure, including the placement relation of V-V, V-O, and O-O.

Methods and Materials: The commercial v2o3 power, (alfa aesar 95% assay), under the additional heat treatment of 300°C in H_2 atmosphere, was used in the experiment. Rietveld refinement is performed to get the average structure and pair-distribution function (PDF) to get the local structure,

Results: The PDF patterns of the low temperature monoclinic phase and high temperature trigonal phase are similar, which shows the local structure of both phases does not change. The diffraction pattern shows an obvious difference, which shows the difference of average global structure

Conclusions: The local structures of both phase the same, which cannot be explained by the pure orbital occupation of Mott-Hubbard type of transition. Other interaction, including spin-spin correlation, electron- spin correlation may take an important role in the metal-insulator transition.

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References: N.F. Mott, Metal – Insulator Transition, 2nd ed. (Taylor & Francis, London, 1990) p. 176.
A.I. Frenkel *et al*., Metal – insulator translation and local structure of V_2O_3, Journal de physique IV C2, 1997, p1061.

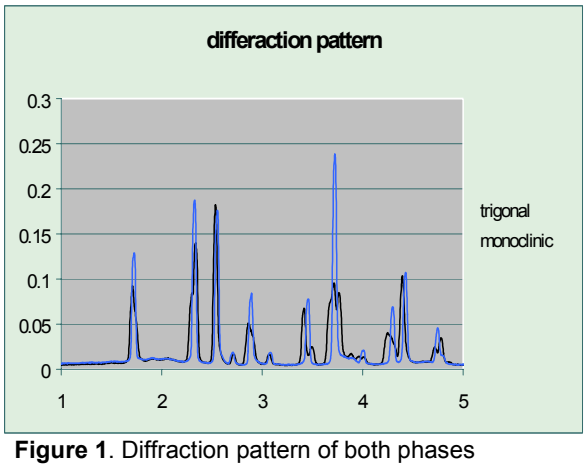

Figure 1. Diffraction pattern of both phases

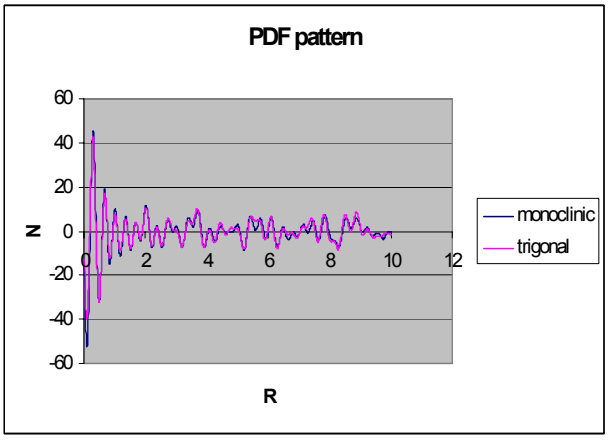

Figure 2. PDF pattern of both phases